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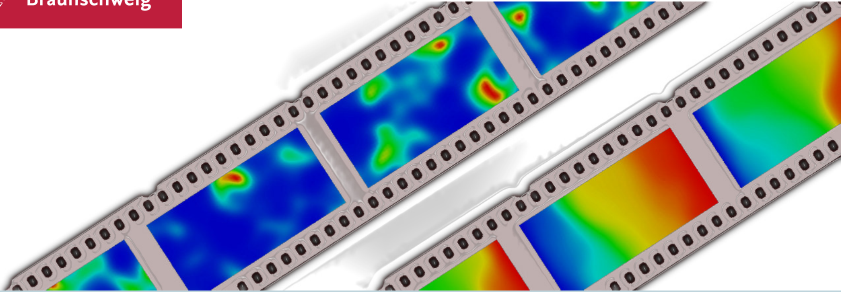

Successive Rank-One Updates and an Adaptive Construction of the Solution Space

Presentation in the course "Uncertainty Quantification, Parametric Problems, and Model Reduction" (INF-WR-014)

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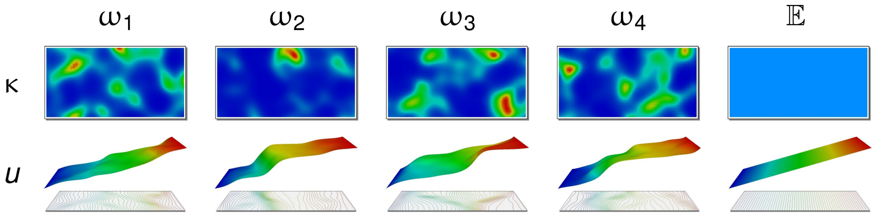
Content

Stationary Groundwater Flow

$$-\nabla_X \cdot \big(\, \kappa(\boldsymbol{x}, \omega)\, \nabla_X u(\boldsymbol{x}, \omega) \,\big) = f(\boldsymbol{x})$$

- $\boldsymbol{x} \in X \subset \mathbb{R}^2, \quad \omega \in \Omega, \quad \mathcal{P} := (\Omega, \mathcal{F}, P)$
- hydraulic conductivity $\kappa : X \times \Omega \to \mathbb{R}$
- uncertain $\kappa \Rightarrow$ uncertain hydraulic head $u : X \times \Omega \to \mathbb{R}$



Discretisation of a Random Field

$$\nu(\boldsymbol{x},\omega) \;\approx\; \nu_h(\boldsymbol{x},\omega) := \sum_{i\in\{1,\dots,N_X\},\, j\in\{1,\dots,N_S\}} \nu_{i,j}\,\phi_i(\boldsymbol{x})\,\psi_j(\omega) \;=\; \boldsymbol{\phi}(\boldsymbol{x})^T \boldsymbol{V}\,\boldsymbol{\psi}(\omega)$$

$$\boldsymbol{V} := \begin{pmatrix} \nu_{1,1} & \cdots & \nu_{1,N_S} \\ \vdots & \ddots & \vdots \\ \nu_{N_X,1} & \cdots & \nu_{N_X,N_S} \end{pmatrix}$$

spatial basis functions $\boldsymbol{\phi} := (\phi_1,\dots,\phi_{N_X})^T$
stochastic basis functions $\boldsymbol{\psi} := (\psi_1,\dots,\psi_{N_S})^T$

- e.g. polynomial chaos expansion (PCE):

$$\psi_i(\omega) := \psi_i(\theta(\omega)), \qquad \psi_i \perp \psi_j \ \ (i \neq j)$$

- $\boldsymbol{V}$ may become large $\Rightarrow$ sparsification of $\boldsymbol{\psi}$?
  low-rank representation of $\boldsymbol{V}$?

A Low-Rank Representation of a Random Field

$$v_h(\boldsymbol{x},\omega) := \phi(\boldsymbol{x})^T \boxed{\boldsymbol{V}} \psi(\omega)$$

$$\approx \quad v_h^r(\boldsymbol{x},\omega) := \phi(\boldsymbol{x})^T \boxed{\sum_{i=1}^{r} \boldsymbol{g}_i \, \boldsymbol{h}_i^T} \psi(\omega) = \phi(\boldsymbol{x})^T \boxed{\boldsymbol{G}\,\boldsymbol{H}^T} \psi(\omega)$$

$$\boldsymbol{G} \in \mathbb{R}^{N_X \times r}, \ \boldsymbol{H} \in \mathbb{R}^{N_S \times r}, \quad r \ll \min\{N_X, N_S\}$$

- reduction of memory requirements
- more efficient computational handling
- e.g. Karhunen-Loève expansion (KLE)

Stochastic Galerkin Method (SGM): Discretisation

A stationary groundwater flow:

$$-\nabla_X \cdot \left(\kappa(\boldsymbol{x},\omega)\, \nabla_X u(\boldsymbol{x},\omega) \right) = f(\boldsymbol{x})$$

Discretising the weak form by

$$u_h(\boldsymbol{x},\omega) \;:=\; (\boldsymbol{\psi}(\omega) \otimes \boldsymbol{\phi}(\boldsymbol{x}))^T \boldsymbol{u} \;=\; \boldsymbol{\phi}(\boldsymbol{x})^T \boldsymbol{U}\, \boldsymbol{\psi}(\omega) \quad \text{(PCE+FE)}$$

leads to a linear system (to be solved):

$$\boxed{\left(\sum_{i=1}^{l} \Delta_i \otimes \boldsymbol{K}_i\right)\boldsymbol{u} = \boldsymbol{f}} \iff \boxed{\sum_{i=1}^{l} \boldsymbol{K}_i \boldsymbol{U} \Delta_i = \boldsymbol{F}} \iff \boxed{\mathcal{A}(\boldsymbol{U}) = \boldsymbol{F}}$$

$\boldsymbol{u}, \boldsymbol{f} \in \mathbb{R}^{N_X \cdot N_S}$ $\qquad$ $\boldsymbol{U}, \boldsymbol{F} \in \mathbb{R}^{N_X \times N_S}$

Successive Rank-1 Updates

Proper Generalised Decomposition (PGD):

- low-rank representation through successive rank-1 updates:
  rank-one update $\boldsymbol{U} = \boldsymbol{U}^{-} + \boldsymbol{g}\boldsymbol{h}^{T} = \boldsymbol{G}^{-}(\boldsymbol{H}^{-})^{T} + \boldsymbol{g}\boldsymbol{h}^{T}$
- locally optimal (greedy)
- not necessarily globally optimal
- not necessarily orthogonal rank-1 updates

Successive Rank-1 Update Scheme (SR1U):

- successive rank-1 updates similar to PGD (greedy)
- optimisation to obtain globally optimal representation (optional)
- not necessarily orthogonal rank-1 updates
- adaptive construction of the stochastic solution space (optional)

Successive Rank-1 Update Scheme (SR1U)

Minimisation of the expectation of the total potential energy:

$$\mathcal{A}(\boldsymbol{U}) = \boldsymbol{F}$$

$$\Longleftrightarrow \quad \boxed{\mathcal{E}(\boldsymbol{U}) \; := \; \frac{1}{2}\mathcal{A}(\boldsymbol{U}) : \boldsymbol{U} - \boldsymbol{F} : \boldsymbol{U} \;\longrightarrow\; \text{min}}$$

with $A : B := \sum_{i,j} A_{ij} B_{ij}, \quad A, B \in \mathbb{R}^{n_1 \times n_2}$

Ansatz:

$$\boxed{\boldsymbol{U} = \boldsymbol{U}^{-} + \boldsymbol{g}\boldsymbol{h}^{T}}$$

(locally optimal rank-1 update)

spatial part $\boldsymbol{g}$

stochastic part $\boldsymbol{h}$

SR1U: Derivation

Differentiating $\mathcal{E}(\boldsymbol{U})$ with respect to $\boldsymbol{U}$ and...

- differentiating $\boldsymbol{U}$ with respect to $\boldsymbol{g}$ leads to (spatial system)

$$\boxed{\boldsymbol{P}(\boldsymbol{h})\ \boldsymbol{g} \;=\; \boldsymbol{b}(\boldsymbol{h})}$$

- differentiating $\boldsymbol{U}$ with respect to $\boldsymbol{h}$ leads to (stochastic system)

$$\boxed{\boldsymbol{Q}(\boldsymbol{g})\ \boldsymbol{h} \;=\; \bar{\boldsymbol{b}}(\boldsymbol{g})}$$

- alternating iterative process

Output: $\boldsymbol{U} := \sum_{i=1}^{r} \boldsymbol{g}_i\ \boldsymbol{h}_i^T \;=\; \boldsymbol{G}\ \boldsymbol{H}^T$

SR1U: Algorithm

```
H ← ∅,    G ← ∅
while break criterion not reached do
    h ← rand,    g ← 0
    while break criterion not reached do
        h ← normalise h
        g ← solve   P(h) g = b(h)
        g ← normalise g
        h ← solve   Q(g) h = b̄(g)
    end while
    G ← [G, g]
    H ← [H, h]
end while
```

SR1U: Solving the Spatial System

$$\boxed{\boldsymbol{P}(\boldsymbol{h})\,\boldsymbol{g} = \boldsymbol{b}(\boldsymbol{h})} \quad \text{with} \quad \boldsymbol{P}(\boldsymbol{h}) := \sum_{i=0}^{l} \underbrace{\boldsymbol{h}^T \Delta_i \boldsymbol{h}}_{=:d_i(\boldsymbol{h})} \boldsymbol{K}_i,$$

$$\boldsymbol{b}(\boldsymbol{h}) := \left(\boldsymbol{F} - \mathcal{A}(\boldsymbol{U}^-)\right) \boldsymbol{h}$$

If $\boldsymbol{K}_i := \boldsymbol{K}(\kappa_i)$ is linear in its material κ_i the computational costs can be reduced:

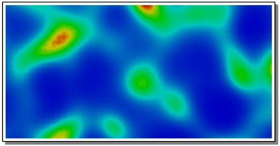
$$\boldsymbol{P}(\boldsymbol{h}) := \sum_{i=0}^{l} d_i(\boldsymbol{h})\,\boldsymbol{K}(\kappa_i) = \boxed{\boldsymbol{K}(\Sigma_{i=0}^{l} d_i(\boldsymbol{h})\,\kappa_i)}.$$

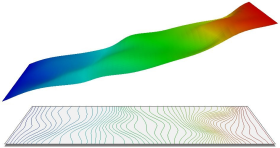
Then, the spatial system may be solved by a simulation code for deterministic models.

SR1U: Stationary Groundwater Flow

Discretisation:

- 5 stochastic dimensions
- 126 stochastic DoFs
- 231 spatial DoFs

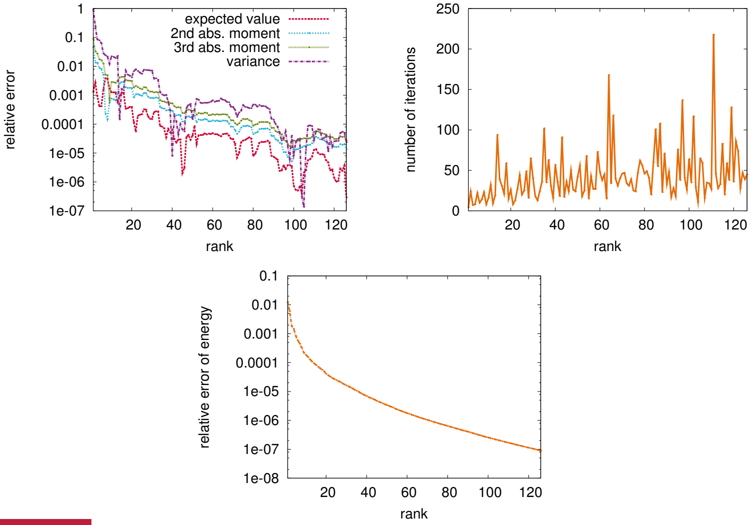




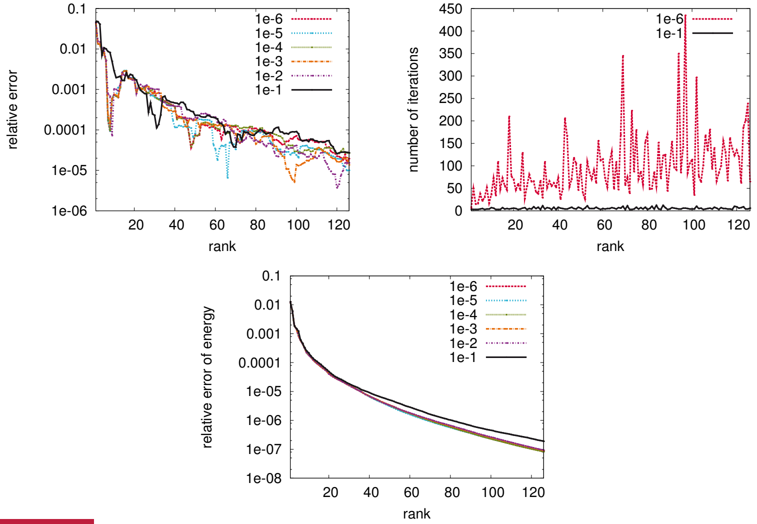
Reference:

- direct solution of the SGM-discretised system

SR1U: Stationary Groundwater Flow (2)



SR1U: Stationary Groundwater Flow (3)



SR1U: Low-Rank Optimisation (OPT)

Improve computed low-rank approximation:

Apply the SR1U scheme onto projections of $\mathcal{A}(\boldsymbol{U}) = \boldsymbol{F}$

$$\begin{aligned} \mathcal{A}(\boldsymbol{U})\boldsymbol{H} &= \boldsymbol{F}\boldsymbol{H} \\ \boldsymbol{G}^T\mathcal{A}(\boldsymbol{U}) &= \boldsymbol{G}^T\boldsymbol{F} \end{aligned}$$

to obtain rank-1 updates

$$\begin{aligned} \boldsymbol{G} &= \boldsymbol{G}^- + \boldsymbol{g}\boldsymbol{v}^T &= \boldsymbol{G}^- + \Delta\boldsymbol{G} \\ \boldsymbol{H} &= \boldsymbol{H}^- + \boldsymbol{h}\boldsymbol{w}^T &= \boldsymbol{H}^- + \Delta\boldsymbol{H} \end{aligned}$$

- a coupled system for each update
- updates without a rank increase for $\boldsymbol{U} = \boldsymbol{G}\,\boldsymbol{H}^T$

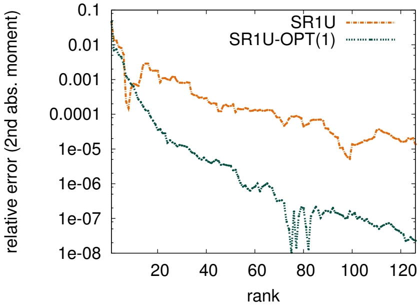
OPT: Algorithm

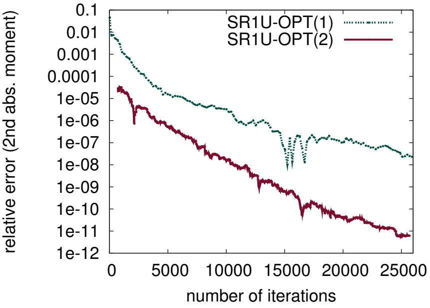
$\boldsymbol{G} \leftarrow \boldsymbol{G}^{-}, \quad \boldsymbol{H} \leftarrow \boldsymbol{H}^{-}$
while break criterion not reached **do**
  $\boldsymbol{g}, \boldsymbol{v} \leftarrow$ get rank-1 update for $\boldsymbol{G}$
  $\boldsymbol{G} \leftarrow \boldsymbol{G} + \boldsymbol{g}\boldsymbol{v}^T$
  $\boldsymbol{h}, \boldsymbol{w} \leftarrow$ get rank-1 update for $\boldsymbol{H}$
  $\boldsymbol{H} \leftarrow \boldsymbol{H} + \boldsymbol{h}\boldsymbol{w}^T$
end while

- accepts arbitrary low-rank inputs
- embedded in the SR1U scheme:
  - on the fly (SR1U-OPT-1)
  - as a post-processor (SR1U-OPT-2)

SR1U-OPT: Stationary Groundwater Flow

Optimise $\boldsymbol{U} = \boldsymbol{G}\,\boldsymbol{H}^T$:





Adaptive Choice of Stochastic Basis Polynomials

Given: $\boldsymbol{U} \quad \Longleftarrow \quad \sum_{i=0}^{l} \boldsymbol{K}_i \boldsymbol{U} \boldsymbol{\Delta}_i = \boldsymbol{F}$

- $\boldsymbol{U}$ is not accurate enough?
- extend the solution space by relevant stochastic polynomials
- recompute $\boldsymbol{U}$

How to find relevant stochastic polynomials?

- add new stochastic polynomials ψ^+: $\quad \boldsymbol{\Delta}_i^{\oplus} := \left(\begin{array}{c|c} \boldsymbol{\Delta}_i & \boldsymbol{\Delta}_i^{\triangleleft} \\ \hline \boldsymbol{\Delta}_i^{\triangleright} & \boldsymbol{\Delta}_i^{+} \end{array} \right)$
- compute the extended residual with current solution $\boldsymbol{U}$

$$\boldsymbol{R}^{\oplus} := \boldsymbol{F}^{\oplus} - \sum_{i=0}^{l} \boldsymbol{K}_i \, \boldsymbol{U} \, \boldsymbol{\Delta}_i^{\uplus} \quad \text{with} \quad \boldsymbol{\Delta}_i^{\uplus} := [\boldsymbol{\Delta}_i, \boldsymbol{\Delta}_i^{\triangleleft}]$$

- rate the new stochastic polynomials and keep the best rated ones

SR1U-ADAPT: Adaptive Solution Space Construction

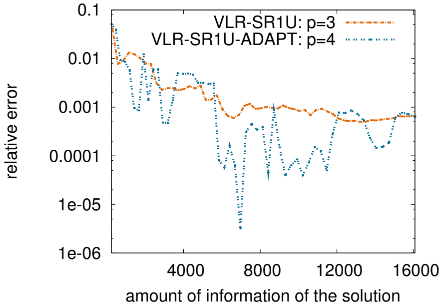
Embedding in the SR1U scheme:

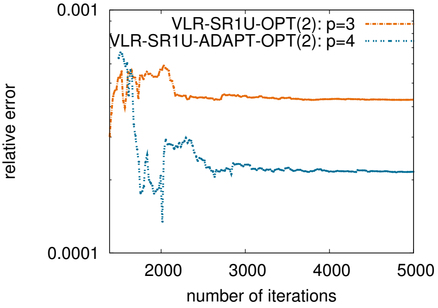
Inout: ψ

1: **if** solution space not fine enough **then**
2: select ψ^+
3: $\hat{\psi} \leftarrow$ rate ψ^+
4: $\psi \leftarrow [\psi, \hat{\psi}]$
5: **end if**

- use the extended solution space for the next rank-1 updates
- one optimisation step takes the previous rank-1 updates to the extended solution space
- no recomputation of $\boldsymbol{U}$ required

SR1U-ADAPT: Stationary Groundwater Flow





SR1U: Intermediate Conclusions

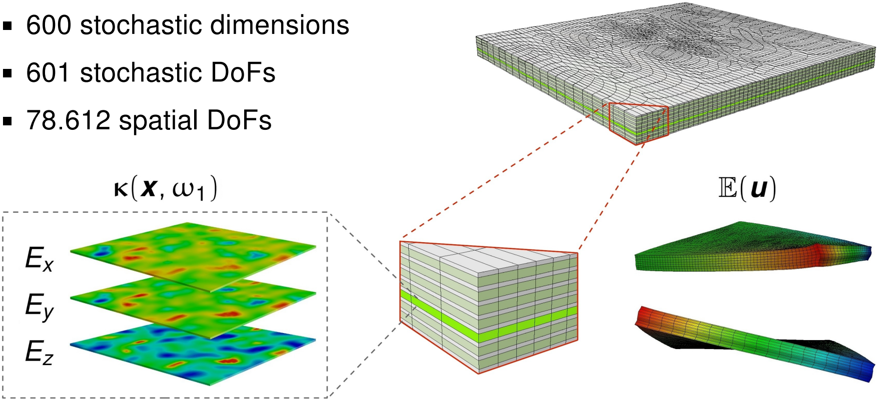
- computational advantage when the stiffness matrix is linear in its material
- few iterations are enough to obtain an accurate rank-1 update
- an optimisation on the fly is less efficient than an optimisation at a final rank
- the residual-based adaption of the stochastic solution space is promising

Laminated Composite Structure with a Linear Constitutive Law

$\kappa : X \times \Omega \to \mathbb{R}^{21}, \quad \boldsymbol{u} : X \times \Omega \to \mathbb{R}^3$

Discretisation:

- 600 stochastic dimensions
- 601 stochastic DoFs
- 78.612 spatial DoFs

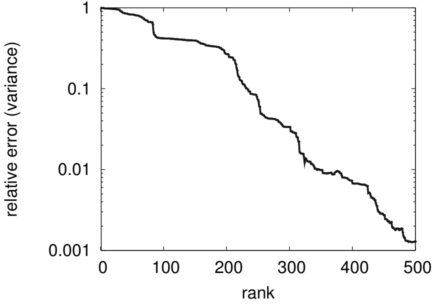


SR1U: Laminated Composite Structure

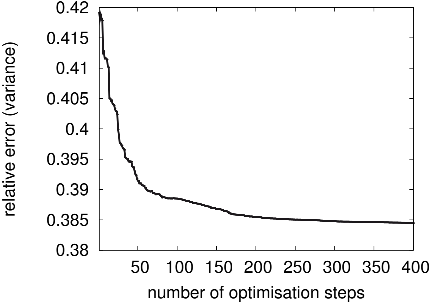
Reference:

- full rank representation (SR1U)

SR1U:



OPT-2 at rank 100:



Summary

Successive rank-1 update scheme:

- in its basic form suboptimal
- optimisation of rank-r solutions
- construction of a sparse stochastic solution space
- convergence for simple and difficult examples

Related Publications:

Martin Krosche. *A Generic Component-Based Software Architecture for the Simulation of Probabilistic Models*. PhD thesis, Technische Universität Braunschweig, Braunschweig, 2013. http://www.digibib.tu-bs.de/?docid=00052792.

Martin Krosche and Rainer Niekamp. Low rank approximation in spectral stochastic finite element method with solution space adaption. Informatikbericht 2010–03, Institut für Wissenschaftliches Rechnen, Technische Universität Braunschweig, Braunschweig, 2010. http://www.digibib.tu-bs.de/?docid=00036351.

Outlook

Successive rank-1 update scheme:

- improve initial guesses for rank-1 updates
- automatic control of rank-1 updates and solution space adaptions
- application to nonlinear problems